2-hydroxy-2,4,4-trimethylpentanoic acid
5438-26-6 | DTXSID90280379

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.13e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.45e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

Image not found
2-Ethoxyethyl isobutyrate
Measured: 1.35e-11
Predicted: 1.28e-11

Image not found
Bornyl acetate
Measured: 1.39e-11
Predicted: 1.36e-11

Image not found
Ethyl 3-ethoxypropionate
Measured: 2.29e-11
Predicted: 1.63e-11

Image not found
Ethyl lactate
Measured: 3.90e-12
Predicted: 4.80e-12

Image not found
Butyl butyrate
Measured: 1.06e-11
Predicted: 1.06e-11